

Efficient numerical solution to vacuum decay with many fields

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Abstract. Finding numerical solutions describing bubble nucleation is notoriously difficult in more than one field space dimension. Traditional shooting methods fail because of the extreme non-linearity of field evolution over a macroscopic distance as a function of initial conditions. Minimization methods tend to become either slow or imprecise for larger numbers of fields due to their dependence on the high dimensionality of discretized function spaces. We present a new method for finding solutions which is both very efficient and able to cope with the non-linearities. Our method directly integrates the equations of motion except at a small number of junction points, so we do not need to introduce a discrete domain for our functions. The method, based on multiple shooting, typically finds solutions involving three fields in under a minute, and can find solutions for eight fields in about an hour. We include a numerical package for Mathematica which implements the method described here.

Contents

1	Introduction	1
2	$O(4)$ bounce formalism	2
3	Solution techniques	3
4	Description of the method	5
4.1	Multiple shooting method	5
4.2	Analytic solutions	7
4.2.1	Analytic solution for large r	7
4.2.2	Analytic solutions near the center of the bounce	8
4.3	Adding a new variable	8
4.4	Readjusting r values	9
4.5	Choice of the initial profile	9
4.6	Calculation of the action	10
5	Examples of potentials solved by the code	11
6	Comparison with other methods	12
6.1	Range of application	12
6.2	Success fraction	13
6.3	Speed	13
6.4	Quality of solution	13
7	Possible issues	13
8	Conclusion	14
A	Calculation of Jacobian	14
A.1	Solving for Jacobian along the path	14
A.2	Jacobian with respect to Δ	15
B	Powell’s method for solving equations	16
C	Obtaining and running the code	17

1 Introduction

The thermal or quantum mechanical nucleation of bubbles initiates a first-order phase transition. This phenomenon has application in diverse areas of physics including superfluid Helium-3 [1, 2], Higgs-induced vacuum decay, [3–7], baryogenesis and gravitational waves from a first-order electroweak phase transition [8–15], and quantum gravitational instabilities [14, 16, 17]. The idea that the observable universe represents but one vacuum [18, 19] in a diverse landscape of string vacua [20, 21] motivates a study of false vacuum decay in high-dimensional field spaces [22–29].

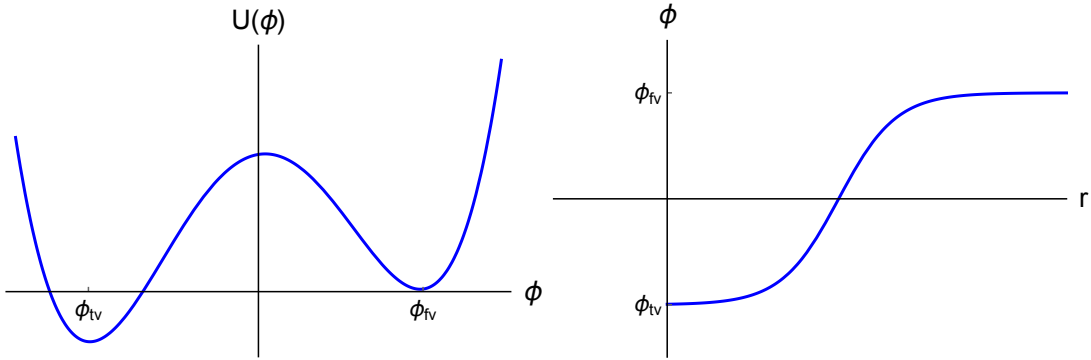


Figure 1. Left panel shows a potential with two vacua. The left vacuum ϕ_{tv} is stable and denoted as the “true vacuum.” The right vacuum ϕ_{fv} , which is meta-stable, is called the “false vacuum.” Right panel shows the field profile that carries the tunneling.

Quantum field theories with an effective potential $U(\phi)$ have perturbatively stable vacua corresponding to the local minima of $U(\phi)$. Non-perturbative effects can destabilize these local minima via the spontaneous nucleation of bubbles containing a lower energy perturbative vacuum [30]. Instanton methods [31, 32] provide a simple and elegant treatment of this process. The primary calculation is a Euclidean $O(4)$ -symmetric “bubble” field profile (called the bounce) which smoothly interpolates between a true-vacuum configuration at its center and the false vacuum whose decay is being described. Once this is calculated, the decay rate follows, as well as the field configuration for the formation and evolution of a single bubble.

This paper is structured as follows. We briefly review the bounce formalism in section 2. In section 3 we describe simple algorithms for finding the bounce solution, and the problems they face. In section 4 we describe our more robust method for finding the bounce. In section 5 we provide examples. In section 6 we compare our method with other methods. In section 7 we describe known or possible limitations to the types of problems our code can currently solve. We conclude in section 8.

2 $O(4)$ bounce formalism

In this section we follow Coleman [31]. We start from the Lagrangian for a scalar field in flat space,

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - U(\phi) , \quad (2.1)$$

where $U(\phi)$ is a potential with two minima. An example is shown in Figure 1. The tunneling is described by a solution to the Euclidean ($x_0 \rightarrow -i\tau$) equations of motion,

$$\nabla^2 \phi = \frac{\partial U}{\partial \phi} . \quad (2.2)$$

Assuming that the field has an $O(4)$ symmetry, i.e., $\phi(x) = \phi(r)$ where $r = \sqrt{\tau^2 + \sum x_i^2}$, (2.2) simplifies to

$$\frac{d^2 \phi}{dr^2} + \frac{D-1}{r} \frac{d\phi}{dr} = \frac{\partial U}{\partial \phi} , \quad (2.3)$$

where D is the number of spacetime dimensions. This is the equation of motion for a particle that moves in the “upside-down” potential $-U(\phi)$ under the influence of the velocity-dependent “friction” term $(D-1)/r$. The boundary conditions are

$$\phi'(0) = 0, \quad \lim_{r \rightarrow \infty} \phi(r) = \phi_{\text{fv}}, \quad (2.4)$$

where the prime denotes differentiation with respect to r .

It is the friction that allows the field to roll to a stop atop the false-vacuum hill, which is lower than the true-vacuum initial position. Since friction weakens inversely with the time parameter r , beginning too close to the peak of the true-vacuum hill will result in a large initial delay, and so too little friction when velocities are large; the field will overshoot the false vacuum.

The simplest non-constant solution with the above properties is known as the bounce. A typical potential and the corresponding bounce field profile are shown in Figure 1. The tunneling rate is given by $\Gamma = Ae^{-B}$, where B is the Euclidean action of the corresponding bounce minus the action of the false vacuum configuration.

Generalization of this problem to more than one field is straightforward. We denote the fields by $\phi = (\phi_1, \phi_2, \dots, \phi_N)$ and the potential by $U(\phi)$. The bounce is then a solution to the system of coupled ordinary differential equations

$$\frac{d^2 \phi_i}{dr^2} + \frac{D-1}{r} \frac{d\phi_i}{dr} = \frac{\partial U}{\partial \phi_i}, \quad (2.5)$$

with boundary conditions $d\phi/dr|_{r=0} = 0$ and $\lim_{r \rightarrow \infty} \phi(r) = \phi_{\text{fv}}$. This is a system of N second-order equations with N boundary conditions at $r = 0$ and another N at $r = \infty$. The field must begin at $r = 0$ from some specific point at the center of the bubble and asymptotically approach the false vacuum infinitely far away. Finding the solution to the bounce equations is tantamount to determining the values of fields at $r = 0$.

For a single field, Coleman [31] used an overshoot-undershoot argument to prove that there is always a bounce that connects a higher meta-stable vacuum to an adjacent lower energy vacuum. However, with more than one field there are cases where no solution exists, as shown, for example, in figure 2.

There are also cases that have more than one solution. With more than one field, there may be more than one “mountain pass” connecting the two vacua, as in figure 7 below. Each pass gives rise to its own instanton. Even with only one field, there are cases with multiple solutions. One example is shown in figure 3, where we drew the upside down potential. Regions shown in red overshoot the true vacuum, while those shown in black undershoot. Thus the right edge of the upper red region and the two edges of the lower red region are each a solution.

For a thermally induced first-order phase transition the formalism is quite similar [1, 32].

3 Solution techniques

The most straightforward method to find the bounce numerically would be shooting from the initial condition $\phi(0) = \phi_0$. Starting from some guess for ϕ_0 , we could integrate the equations of motion to large r . The correct value of ϕ_0 yields the desired asymptotic boundary condition $\phi \rightarrow \phi_{\text{fv}}$. We could iteratively improve ϕ_0 based on how close ϕ comes to ϕ_{fv} .

This technique requires integrating the differential equation (2.5) from $r = 0$ to large r . For a single field, so long as we are descending the inverted potential from the true vacuum,

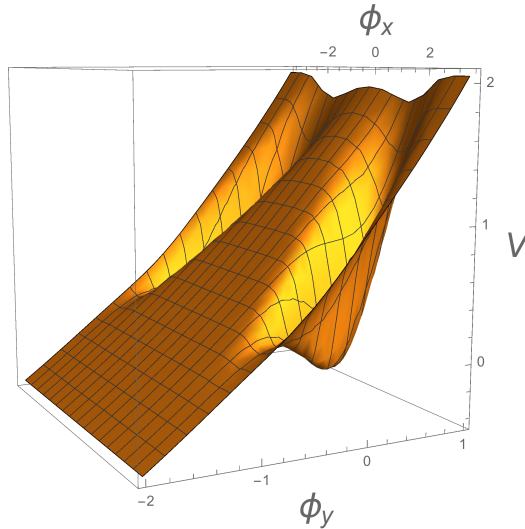


Figure 2. In this two-dimensional potential there is no instanton connecting the two minima on the right. The problem is that tunneling between the two minima is dominated by tunneling to lower values on the left.

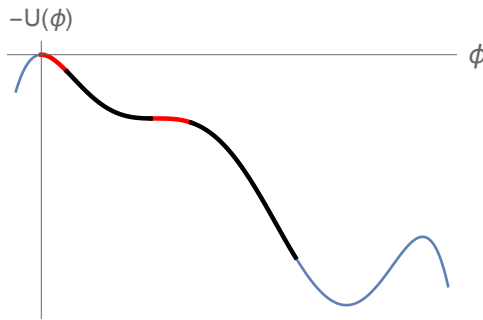


Figure 3. A one-dimensional potential, shown inverted, that has more than one solution.

this equation is stable. But as we ascend the inverted potential toward the false vacuum, it becomes unstable. The desired solution asymptotically approaches ϕ_{fv} , but there is another solution which more and more rapidly falls down the hill. This growing mode causes numerical instability that makes it impossible to find the solution with the correct $\phi \rightarrow \phi_{\text{fv}}$ boundary condition.

This problem can be avoided by a “double shooting” scheme [33]. We pick ϕ_0 as above and pick also some large but finite value r_{max} and a field value $\phi(r_{\text{max}}) = \phi_{\text{max}}$ there. Then we integrate (2.3) to the right from $r = 0$ and to the left from r_{max} , and demand that the two solutions match at some intermediate location. We then attempt to iteratively improve ϕ_0 and ϕ_{max} .

The double shooting technique works reasonably well for one field, but for additional fields we face additional problems. One problem is that the solution may travel along a “ridge” in the inverted potential. In this case, there is an unstable mode that falls off the ridge instead of traveling along it. Reversing the direction of integration does not help this problem.

This problem exists even when the field is descending the inverted potential. Unless it is following the steepest descent, modes that descend in steeper directions will always be more

unstable than the desired mode. This occurs even near the true and near the false vacuum.

A related problem is that in many cases, ϕ_0 can never be specified with sufficient accuracy. For example, consider a potential which near the true vacuum has the form

$$U(\phi_1, \phi_2) = 10(\phi_1^2 + \phi_2^2) - 16\phi_1\phi_2. \quad (3.1)$$

Neglecting friction, the solution is

$$\phi_1 = Ae^{2r} + Be^{6r}, \quad (3.2)$$

$$\phi_2 = Ae^{2r} - Be^{6r}. \quad (3.3)$$

Suppose we want to reach $\phi = (2, 0)$ at $r = 10$. Then we need $A = e^{-20}, B = e^{-60}$, and thus $\phi_0 = (e^{-20} + e^{-60}, e^{-20} - e^{-60})$. But in double-precision floating point, $e^{-20} \pm e^{-60}$ is indistinguishable from e^{-20} , so we end up with $\phi_0 = (e^{-20}, e^{-20})$, and thus $\phi(10) = (1, 1)$ instead of $(2, 0)$. Including the friction term would lead to Bessel functions instead of exponentials, but the effect is the same.

4 Description of the method

As mentioned in section 2, the simple shooting methods for solving the bounce equations face several difficulties, which we address here. The most significant problem is solving a set of differential equations that are unstable. We overcome this problem using a multi-interval shooting method described in subsection 4.1. At the center of the bubble ($r = 0$) there is a divergence in (2.5). Additionally, the other boundary condition is set at $r = \infty$, which clearly cannot be represented in machine precision. We solve these problems by using an approximate analytic solution in subsection 4.2. In subsection 4.3 we add an additional variable to the set for which we are solving, in order to make it easier for the system to change the solution by translation in r , and in subsection 4.4 we make changes to the division points between the shooting regions.

To find the bounce solution using shooting methods we need to come up with an initial guess. The procedure for finding a good initial guess is described in subsection 4.5. After we find the solution, we need to calculate the action, which is discussed in subsection 4.6.

Solving non-linear equations using steepest decent guarantees that the steps taken toward the solution are small, but this method converges slowly. On the other hand Newton's method converges rapidly, but can take dangerously large steps. We use Powell's hybrid method, which converges quickly near the solution, yet takes reasonable steps far away from it. This is explained in appendix B. To use this method we need to calculate the Jacobian of the field values with respect to the initial conditions. We use an accurate method for calculating the Jacobian which is described in appendix A. Appendix C explains how to download and run the code.

4.1 Multiple shooting method

The differential equations (2.5) are unstable in the sense that there are growing and decaying modes, and the growing modes may have different rates of growth. Unless we are interested in the fastest mode, a small admixture of this mode from numerical error will eventually overpower the solution of interest. To avoid this problem, we integrate the differential equations only over a range of r small enough that the growth is tolerable, and put together several such regions to cover the needed range of r . This method is known as multiple shooting [34].

To understand the degree of instability, let us expand $U(\phi)$ around some specific point ϕ_1 to quadratic order,

$$U(\phi) = U(\phi_1) + A_i(\phi - \phi_1)_i + (B_{ij}/2)(\phi - \phi_1)_i(\phi - \phi_1)_j + \mathcal{O}(\phi - \phi_1)^3, \quad (4.1)$$

where

$$A_i = \left. \frac{\partial U}{\partial \phi_i} \right|_{\phi_1}, \quad B_{ij} = \left. \frac{\partial^2 U}{\partial \phi_i \partial \phi_j} \right|_{\phi_1}. \quad (4.2)$$

If we use (4.2) and ignore the frictional term in (2.5), we have

$$\frac{d^2 \phi_i}{dr^2} = A_i + B_{ij}(\phi - \phi_1)_j. \quad (4.3)$$

We can diagonalize the symmetric matrix B_{ij} using an orthogonal matrix O , so $B_{ij} = O_{ki} \tilde{B}_{kl} O_{lj}$ with $\tilde{B}_{kl} = \text{diag}(B_1, B_2, \dots, B_N)$. Define $\tilde{\phi}_i = O_{ij}(\phi - \phi_1)_j$ and $\tilde{A}_i = O_{ij}A_j$, so that

$$\frac{d^2 \tilde{\phi}_i}{dr^2} = \tilde{A}_i + B_i \tilde{\phi}_i. \quad (4.4)$$

Assuming that all B_i are positive, which is the case near the true and false vacua, but not everywhere, the solutions to (4.4) include a mode that grows as $e^{\sqrt{B_i}r}$ and one that shrinks as $e^{-\sqrt{B_i}r}$. If B_{\max} is the largest of the B_i , then the worst case is that the correct solution goes as $e^{-\sqrt{B_{\max}}r}$, so the fastest-growing mode grows relative to the correct solution as $e^{2\sqrt{B_{\max}}r}$.

Let the domain $r \in [0, \infty)$ be divided by $n \geq 3$ intermediate points, $\{r_1, r_2, \dots, r_n\}$. We discuss the method of choosing these points in subsection 4.5. At each step, our variables are the values of the field at r_1 and r_n and for $n > 3$ the field and its derivative at r_2, \dots, r_{n-2} . Notice that we do not use the value of the field and its derivative at r_{n-1} as variables. As described in the next subsection, we do not solve the differential equation for $r < r_1$ nor $r > r_n$. Instead, in these regions, we approximate the potential by a quadratic and so get an analytic solution for $\phi(r)$, and using this solution we determine $\phi'(r_1)$ and $\phi'(r_n)$. Having the field and derivatives we can do the following numerical integrations of (2.5):

1. Integrate from r_i to r_{i+1} for $i = 1 \dots n-2$ to obtain $\phi_L(r_{i+1})$ and $\phi'_L(r_{i+1})$.
2. Integrate from r_n to r_{n-1} to $\phi_R(r_{n-1})$ and $\phi'_R(r_{n-1})$.

Here ϕ_L and ϕ_R denote the values of these quantities obtained by integrating from the left and from the right, respectively. Since we want a smooth solution to the equations of motion, we try to match the values of ϕ_L and ϕ'_L with the corresponding variables at r_2, r_3, \dots, r_{n-2} and ϕ_L and ϕ'_L with ϕ_R and ϕ'_R at point r_{n-1} . This is shown for $n = 3$ and $n = 4$ in Figure 4.

The problem is now reduced to finding the values of $(2n-4)N$ variables that satisfy $(2n-4)N$ equations. We use Powell's hybrid method, described briefly in appendix B, for this purpose.

The reason for shooting toward the left in the last interval is that in this interval (at least by r_n) the inverted potential is increasing toward the false vacuum. Shooting forward corresponds to going uphill which is unstable in proportion to the largest eigenvalue around the false vacuum, but shooting downhill is only sensitive to the difference between eigenvalues, and hence we reduce the sensitivity of the solution. A possible improvement would be to shoot toward the left for more intervals if the potential is also increasing there, but we don't have any way to know in advance which these will be, and so we did not implement this technique.

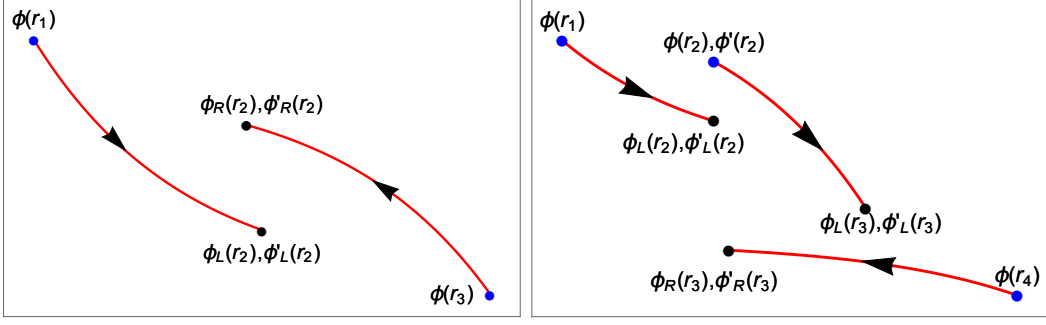


Figure 4. The left panel shows the parameters used when there are only three points. We try to find $\phi(r_1)$ and $\phi(r_3)$ to make $\phi_L(r_2) = \phi_R(r_2)$ and $\phi'_L(r_2) = \phi'_R(r_2)$. The right panel shows the case of four points. Here we try to find $\phi(r_1)$, $\phi(r_2)$, $\phi'(r_2)$, and $\phi(r_4)$ to make $\phi_L(r_2) = \phi(r_2)$, $\phi'_L(r_2) = \phi'(r_2)$, $\phi_L(r_3) = \phi_R(r_3)$, and $\phi'_L(r_3) = \phi'_R(r_3)$.

4.2 Analytic solutions

As described above, we use closed-form solutions to equations with an approximate potential for $r < r_1$ and $r > r_N$. This technique solves the problem where finite numerical accuracy makes it impossible to solve the equations of motion at $\phi = \phi_0$, and another problem where if we integrate the differential equation for sufficiently large r , numerical inaccuracy will always lead to a divergence.

4.2.1 Analytic solution for large r

When the field is very close to the false vacuum, we can approximate $U(\phi)$ with a quadratic. This allows an approximate analytic solution for ϕ . Of the two solutions to the second order field equations, we clearly want the one which approaches a constant as $r \rightarrow \infty$. This enables us to deduce $\phi'(r_n)$ as a function of $\phi(r_n)$. We then use $\phi(r_n)$ and $\phi'(r_n)$ to integrate backward to r_{n-1} and apply the matching conditions there.

So consider r_n large enough so that the fields $\phi(r_n)$ are very close to their false vacuum values. Unless the field has the correct derivative, it will fall off the hill in some direction; for a given $\phi(r_n)$ there is a unique $\phi'(r_n)$ that lands on the hilltop. The potential is given by the expansion (4.1) around ϕ_{fv} , with $A_i = 0$ here, and the equation of motion becomes

$$\frac{d^2 \tilde{\phi}_i}{dr^2} + \frac{D-1}{r} \frac{d\tilde{\phi}_i}{dr} = B_i \tilde{\phi}_i. \quad (4.5)$$

We're interested in the solution which approaches $\tilde{\phi}_i(r) = 0$ as $r \rightarrow \infty$, which is

$$\tilde{\phi}_i(r) = C_i r^{\frac{2-D}{2}} K_{\frac{D-2}{2}} \left(\sqrt{B_i} r \right), \quad (4.6)$$

where $K_{(D-2)/2}$ denotes the Bessel function of type K , and the C_i are constants. Returning to the original field variables,

$$\phi_i(r) = \phi_{\text{fv}i} + \sum_j O_{ji} C_j r^{\frac{2-D}{2}} K_{\frac{D-2}{2}} \left(\sqrt{B_j} r \right). \quad (4.7)$$

For a given $\phi(r_n)$ we determine the C_i and from there calculate $\phi'(r_n)$, which we use to shoot towards r_{n-1} .

4.2.2 Analytic solutions near the center of the bounce

The situation near $r = 0$ is similar. We do not use ϕ_0 as a parameter, but instead use $\phi_1 = \phi(r_1)$. Here we *do not* assume that ϕ_1 is close to the true vacuum, and we expand not around ϕ_{tv} but around ϕ_1 , which is accurate as long as the ϕ_0 that we infer is not too far from ϕ_1 .

The expansion is exactly as in (4.1), and the resulting equation of motion is

$$\frac{d^2 \tilde{\phi}_i}{dr^2} + \frac{D-1}{r} \frac{d\tilde{\phi}_i}{dr} = \tilde{A}_i + B_i \tilde{\phi}_i . \quad (4.8)$$

The initial condition $\tilde{\phi}'_i(0) = 0$ picks out the solution with I -type Bessel functions,

$$\tilde{\phi}_i(r) = C_i r^{\frac{2-D}{2}} I_{\frac{D-2}{2}} \left(\sqrt{B_i} r \right) - \frac{\tilde{A}_i}{B_i} , \quad (4.9)$$

and the requirement that $\phi(r_1) = \phi_1$, so $\tilde{\phi}_i(r_1) = 0$, fixes the C_i , giving

$$\tilde{\phi}_i(r) = \frac{\tilde{A}_i}{B_i} \left[\left(\frac{r_1}{r} \right)^{\frac{D-2}{2}} \frac{I_{\frac{D-2}{2}}(r\sqrt{B_i})}{I_{\frac{D-2}{2}}(r_1\sqrt{B_i})} - 1 \right] . \quad (4.10)$$

In the original field variables,

$$\phi_j(r) = \phi_{1j} + \sum_j O_{ji} \frac{\tilde{A}_j}{B_j} \left[\left(\frac{r_1}{r} \right)^{\frac{D-2}{2}} \frac{I_{\frac{D-2}{2}}(r\sqrt{B_j})}{I_{\frac{D-2}{2}}(r_1\sqrt{B_j})} - 1 \right] . \quad (4.11)$$

Thus from ϕ_1 we can find the derivative $\phi'(r_1)$, and we use these to shoot to r_2 .

4.3 Adding a new variable

A generic field profile of the correct bounce solution (e.g., figure 1) has plateaus at small and large r and a relatively small transition region. However, we do not have any a priori knowledge of the r values near the transition. This leads to an important numerical difficulty. The differential equations in (2.5) exhibit an approximate r -translation symmetry that is broken by the friction term. If $\phi(r)$ is a solution, $\phi(r+\Delta)$ would almost satisfy the differential equation and we will be in a situation depicted in Figure 5. If the code finds a translated version of the field profile, it nearly satisfies the constraints. While the two profiles are simply related by translation in r , in the field variables used in the solution, $\phi(r_1), \phi(r_2), \phi'(r_1), \dots$ the translation is very complicated, requiring adjustment of all variables in a coordinated way. This makes it difficult for the code to make progress after finding the translated profile.

To solve this problem, we add to the variables used by the equation solver an additional variable Δ , representing a translation of the parameters r_i . Instead of using the set of points r_1, r_2, \dots, r_n shown in Figure 4 we use the set of $r_1 + \Delta, r_2 + \Delta, \dots, r_n + \Delta$. Thus changing Δ does not change the values of the fields and derivative variables, but changes the location where these variables are applied, making it simple for the solver to move in the direction of translations in r .

By introducing Δ , we have one more unknown than our equations, so there are infinitely many solutions, but any one is the solution to the problem, expressed in its own way. This method proves to be very effective and extends the range of potentials for which the code can find solutions.

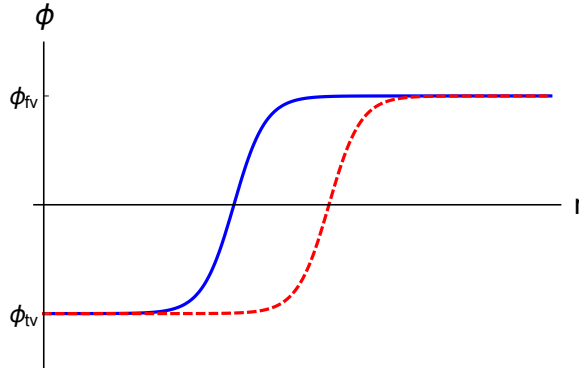


Figure 5. Correct (solid blue) and translated (dashed red) field profiles. If the code finds the translated profile, it may be difficult for it to find the correct profile.

4.4 Readjusting r values

We used approximate analytic solutions in sections 4.2.1 and 4.2.2. For these approximations to be valid, we need r_1 small enough and r_n large enough so that ϕ_1 is close to ϕ_0 and ϕ_n close to ϕ_{fv} . While we construct the initial guess (see section 4.5) so that this is true, later improvement of ϕ_1 and ϕ_n may move these values outside the range that allows for an accurate approximation. Conversely, if ϕ_1 is very close to ϕ_0 or ϕ_n very close to ϕ_{fv} , it means that we can use the analytic solution for larger regions.

To keep ϕ_1 and ϕ_n in the desirable ranges, we use a constant, f_s , giving the permissible distance between ϕ_0 and ϕ_1 and another, f_e , giving the permissible distance between ϕ_n and ϕ_{fv} , both as a fraction of the distance from ϕ_{tv} to ϕ_{fv} . Both constants default to 0.01. If the code reaches distances that are larger, we add new r points below the current r_1 or above the current r_n to the points r_1, \dots, r_n , and if they are much smaller (by factor 10), we remove points from r_1, \dots, r_n and use the analytic solution over a larger range.

4.5 Choice of the initial profile

Probably the most important step in solving a set of equations is choosing an initial point for the solver which is close to the real solution. A bad choice which is out of the basin of attraction would make it impossible to find the solution. When we have more than one field, there are two parts to the initial guess: what path through field space should the initial profile follow, and how should it move along this path as a function of r ?

For the path, by default we simply take a straight line from the true to the false vacuum. But we also allow specification of a set of points $\{\phi_1, \dots, \phi_P\}$ through which the initial solution must go. In this case we draw a smooth curve (a cubic spline, or quadratic if $P = 1$) through the points $\{\phi_{tv}, \phi_1, \phi_2, \dots, \phi_P, \phi_{fv}\}$. We parameterize this path as $\phi_{\text{profile}}(\lambda)$ with $\lambda = 0 \dots 1$.

For the shape of the profile as a function of r , we use an initial guess based on a thin-wall analogy. We first define a one-dimensional potential

$$U_{1d}(\lambda) = U(\phi_{\text{profile}}(\lambda)) + (3\lambda^4 - 4\lambda^3)(U(\phi_{fv}) - U(\phi_{tv})) . \quad (4.12)$$

This modified potential has two degenerate minima at $\lambda = 0$ and $\lambda = 1$ and it shares the same curvature with the original potential at the true vacuum. This potential allows for a

domain-wall solution in the form

$$r(\lambda) = r_0 + \int \frac{d\lambda}{\sqrt{2U_{1d}(\lambda)}} \left| \frac{d\phi_{\text{profile}}}{d\lambda} \right|. \quad (4.13)$$

We chose the constant of integration r_0 so that the field at the half-way path length between true and false vacua is at the radius calculated from thin-wall approximation. The initial profile is then defined by inverting (4.13) and using $\phi_{\text{initial}}(r) = \phi_{\text{profile}}(\lambda(r))$.

Once we have the profile, we need to choose the points r_i . We choose r_1 to be midway from the center to the edge of the region where the analytic approximation can be used, as defined in section 4.4, and similarly r_n midway from the false vacuum to the edge of the final analytic region.

To decide how many r_i values to use, we attempt to make the growth of the field during any shooting region no more than a certain limit, by default a factor of 30. We make the approximation of exponential growth as in section 4.1. Thus the r values should be separated by no more than δr_{max} where $e^{\delta r_{\text{max}} \sqrt{B_{\text{max}}}}$ is the allowable growth and B_{max} the largest eigenvalue of the Hessian matrix. However, since we don't know what values of the field we will use, we choose B_{max} to be the largest eigenvalue of the Hessian in the true or the false vacuum. Having found δr_{max} , we divide the range between r_1 and r_n into the smallest number of equal segments that leads to an interval no more than δr_{max} .

4.6 Calculation of the action

Once we have found the correct profile for the instanton, we would like to find the tunneling action. It is given by

$$S[\phi] = A_{D-1} \int_0^\infty dr r^{D-1} \left[\frac{1}{2} \partial_r \phi_i \partial_r \phi_i + U(\phi) - U(\text{fv}) \right] = S_1 + S_2, \quad (4.14)$$

where A_{D-1} is the area of the unit (D-1)-dimensional sphere, and S_1 is the kinetic term and S_2 the rest. Assuming that $\phi(r)$ is a solution to the equations of motion, we can transform (4.14) in several ways. First, define a family of scale-transformed functions $\phi_\Lambda(r) = \phi(\Lambda r)$. We can calculate the action in (4.14) using $\phi_\Lambda(r)$, following [35],

$$S(\Lambda) = A_{D-1} \int_0^\infty dr r^{D-1} \left[\frac{1}{2} \partial_r \phi_{\Lambda i} \partial_r \phi_{\Lambda i} + U(\phi_\Lambda) - U(\text{fv}) \right] = \Lambda^{2-D} S_1 + \Lambda^{-D} S_2, \quad (4.15)$$

This action must have a stationary point at $\Lambda = 1$, which implies

$$D S_2 = S_1 (2 - D). \quad (4.16)$$

We can also integrate by parts in S_1 . The boundary terms vanish, and we can use the equation of motion (2.5) to find

$$S_1 = -\frac{A_{D-1}}{2} \int_0^\infty dr r^{D-1} \frac{\partial U}{\partial \phi_i} \phi_i. \quad (4.17)$$

Our goal is to give, as much as possible, the action of the correct instanton profile, rather than the action of the actual profile that we found (which is divergent, because our profile has small discontinuities where the shooting regions join). So we are free to make any transformations to the action in terms of the exact profile, and then use the approximate profile in the computation.

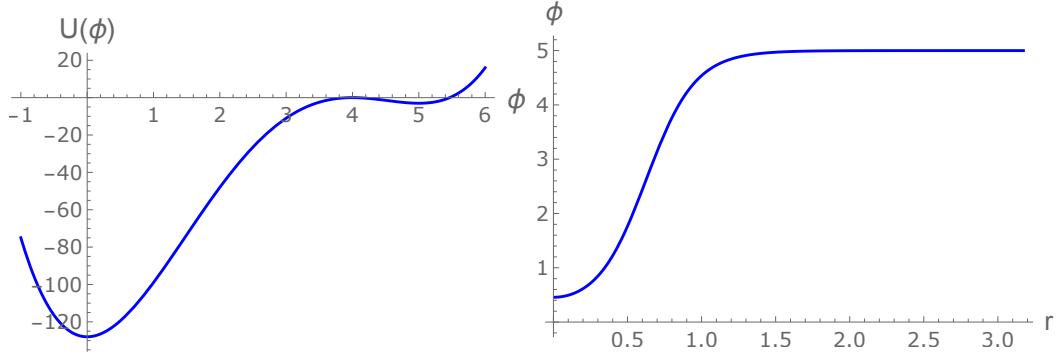


Figure 6. The potential and field profile for the one-dimensional potential given in (5.1). This is an example of a thick-wall solution solved in under four seconds.

Computation using $\partial_r \phi_i$ would be a poor choice, because the derivative is less accurately represented than the function itself in the numerical result of solving the differential equation. We might use (4.16) to write the action in terms of S_2 alone, but this fails when $D = 2$. So instead we use (4.16) to write the action in terms of S_1 alone, and calculate that with (4.17). As long as the profile can be differentiated analytically, using $\partial U / \partial \phi_i$ does not introduce any additional error.

Thus we perform numerically the integral

$$S[\phi] = -\frac{\pi^{D/2}}{\Gamma(1 + D/2)} \int_0^\infty dr r^{D-1} \left[\frac{\partial U}{\partial \phi_i}(\phi(r)) - \frac{\partial U}{\partial \phi_i}(\text{fv}) \right] \phi_i(r) . \quad (4.18)$$

With exact computation, $\partial U / \partial \phi_i$ would vanish at the false vacuum. But numerical error can give a tiny result, which we subtract off explicitly. This prevents it from being amplified into an infinite error under the integral out to $r = \infty$.

5 Examples of potentials solved by the code

Here we show three examples of one, two and three field cases solved using this code. We tried the one-dimensional potential

$$U(\phi) = \phi^4 - 12\phi^3 + 40\phi^2 . \quad (5.1)$$

This potential has minima at $\phi = 0$ and $\phi = 5$, and the code calculated the bounce in under 4 seconds on a Macbook Pro. The potential and solution are shown in Figure 6.

As a two-dimensional example, we solved the bounce solution for the two-field potential given by

$$U(\phi_1, \phi_2) = \sin(\phi_1 - \phi_2) + \frac{1}{2} \cos(\phi_1 + \phi_2) + \cos 3(\phi_1 + \phi_2) + 2 \cos \frac{3}{2}(2\phi_1 - \phi_2) . \quad (5.2)$$

This was solved in ten seconds on a Macbook Pro. The potential and field profiles are shown in Figure 7.

As the last example we show a four field case which took about fifteen minutes to get the solution. The potential is given by

$$\begin{aligned} U = & -1.2 \cos(\phi_1 + 2\phi_2 - \phi_3 - \phi_4) - 1.25 \cos(2\phi_1 - \phi_2 - 2\phi_3 - \phi_4) \\ & - 0.75 \cos(\phi_1 - 2\phi_2 - 2\phi_3 - \phi_4) \\ & - \cos(\phi_1 + \phi_2 - \phi_3 + \phi_4) - 0.5 \cos(\phi_1 - \phi_2 - \phi_3 - 2\phi_4) . \end{aligned} \quad (5.3)$$

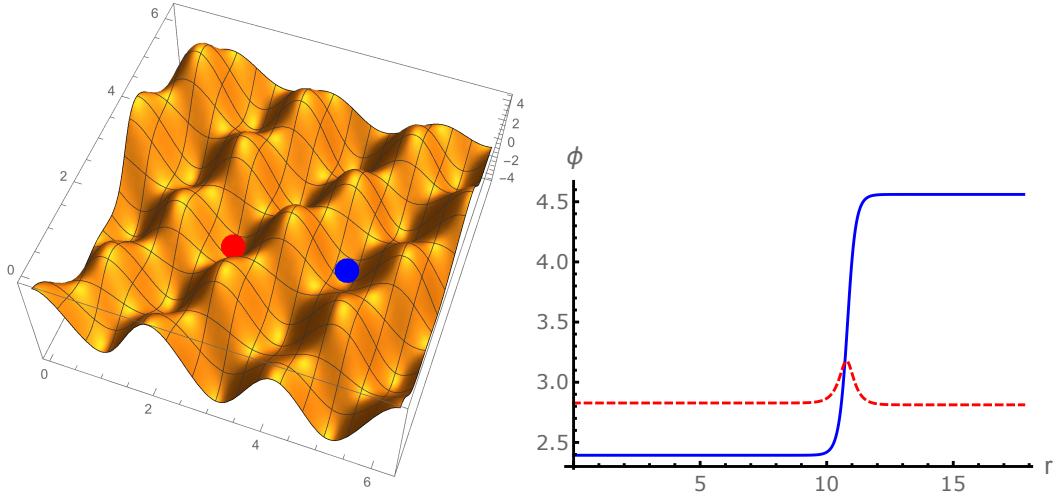


Figure 7. The potential and field profile for the two-dimensional potential given in (5.2). True and false vacua are shown by the red and blue circles. Blue solid and red dashed lines correspond to ϕ_1 and ϕ_2 . The true and false vacua are at (2.39338, 2.82768) and (4.56086, 2.81235).

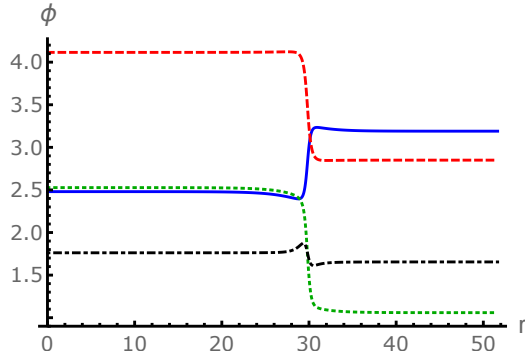


Figure 8. The potential and field profile for the two-dimensional potential given in (5.3). This is an example of a thin-wall solution. The blue solid, red dashed, green dotted and black dot-dashed correspond to ϕ_1, ϕ_2, ϕ_3 and ϕ_4 .

We found the instanton that gives the tunneling from a false vacuum at (3.18979, 2.84979, 1.05933, 1.65474) to a true vacuum at (2.48005, 4.1149, 2.52733, 1.76197). The field profiles are shown in Figure 8.

6 Comparison with other methods

6.1 Range of application

The primary application for our method is vacuum decay in potentials with a large number of fields. We have successfully tested our code on random quartic potentials for $N \leq 9$. We have found bubbles whose radius is larger than the wall thickness by a factor of 200, and extreme thick wall cases, where there is no clear distinction between the interior and the wall.

Ref. [36] reports success for $N = 3$, which is the largest we know of prior to the present work.

6.2 Success fraction

We find that our code succeeds (for $N = 2$) over 99% of the time using the lowest two minima of random quartics¹. For $N = 3$, the success rate was about 97%. In the majority of these cases, the solution was found to 6-digit precision in under 40 seconds. The few that did not complete were in the extreme thin-wall regime, and likely would have succeeded if less accuracy had been sought.

6.3 Speed

Our code finds solutions in a matter of seconds for one to three fields, minutes for four to seven fields, and hours for eight to nine fields. We have not attempted to run our code for ten or more fields.

Most of the time is spent computing the Jacobian. The Jacobian for each shooting region has $4N^2$ elements. These are determined by integrating a matrix differential equation, as discussed in appendix A, which requires matrix multiplication, and thus $8N^3$ operations for each integration step in the differential equation. One could perhaps abandon explicit calculation of the Jacobian in favor of finite differences, or write a special-purpose program for doing the integration. The code could also be run in parallel, at a minimum by handling the different shooting regions on different processors.

6.4 Quality of solution

For solutions not too deep in the thin wall regime, we can test our code against single shooting. In these cases we find that our code agrees with profiles obtained via single shooting to about 10^{-4} . When we decrease the parameters f_s and f_e (defined in section 4.4) by two orders of magnitude compared to their default values of 10^{-2} , the profile error decreases by two orders of magnitude, to 10^{-6} .

Ref. [13, 37] yielded accuracies of order 10^{-2} , and [36] yielded profiles accurate to 10^{-3} . Konstandin & Huber [38] report errors of 2×10^{-4} using 1600 lattice sites.

7 Possible issues

Here we describe certain difficulties the user may encounter with the code. Some of these may be resolved in future releases.

- Runaway potentials (i.e., those whose true vacua do not exist) are not currently supported. Note that it is always possible to modify such potentials, moving the true vacuum in to finite field values, in a way which does not affect the bounce instanton.
- As discussed in subsection 4.2, near the beginning and end of the profile, we use analytic solutions to the potential expanded to second-order in a Taylor series around ϕ_1 and the false vacuum, respectively. For this to work, Mathematica has to be able to compute the second derivative, which causes trouble with certain non-analytic functions such as `Abs`, `UnitStep` and `Norm`. For it to be accurate, there should not be large changes or discontinuities in the Hessian between ϕ_0 and ϕ_1 and between ϕ_n and the false vacuum. It is fine to have a piecewise-defined potential, so long as f_s and f_e are small enough that the boundaries between pieces cannot fall in these regions.

¹We excluded potentials where the lowest two minima were nearly degenerate.

- Potentials whose Hessian has a vanishing eigenvalue at the false vacuum are not supported. A vanishing eigenvalue at a point chosen as r_1 would also be problematic, but this is unlikely ever to occur unless the Hessian eigenvalue vanishes over a non-infinitesimal region.

8 Conclusion

We have presented here a multi-shooting method for the calculation of instantons for the nucleation of bubbles of true vacuum inside a false vacuum in a potential depending on several fields. This method succeeds nearly all the time in the tests that we have done. For one to three fields it runs quite quickly, and even for nine fields it succeeds, albeit slowly.

We have made our Mathematica implementation of this method freely available, as described in appendix C below. We hope it will be useful, both for the calculation of tunneling rates in specific models, and for statistical surveys of large numbers of random potentials.

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A Calculation of Jacobian

In order to implement Powell’s hybrid method we need to know how the equations change when we change the parameters. One way to do so is by changing the parameters by small amounts to see how the result changes. In fact, Powell [39] gives a procedure to do this, primarily using the sequence of parameter choices. However, direct calculation of the Jacobian is more reliable and less prone to numerical errors, and it is possible to do that here.

A.1 Solving for Jacobian along the path

To compute the Jacobian, we need to know, for each shooting step, the way in which the solution to the differential equation, and thus the value of the field and its derivative at the endpoint, depend on the initial conditions.

We start with a system of first order differential equations,

$$\mathbf{f}'(r) = \mathbf{F}(r, \mathbf{f}(r)) , \quad (\text{A.1})$$

with the initial conditions $\mathbf{f}(0)$ given. That is, $\mathbf{f}(r)$ is a vector function of r whose derivative depends upon r and the value of \mathbf{f} at r . We want to know how the solution of the differential equation at some point r depends on changes to the initial conditions. So suppose that we start with infinitesimally different initial conditions $\mathbf{g}(0)$. Assuming \mathbf{F} is a smooth function, these new conditions will give rise to an infinitesimally different solution $\mathbf{g}(r)$ and we can define $\mathbf{A}(r) = \mathbf{g}(r) - \mathbf{f}(r)$. Then \mathbf{A} satisfies a simple differential equation,

$$\mathbf{A}'(r) = \mathbf{g}'(r) - \mathbf{f}'(r) = \mathbf{F}(r, \mathbf{g}) - \mathbf{F}(r, \mathbf{f}) = \mathbf{F}(r, \mathbf{f} + \mathbf{A}) - \mathbf{F}(r, \mathbf{f}) = \frac{\partial \mathbf{F}}{\partial f_j} A_j(r) . \quad (\text{A.2})$$

The first-order effect on $f_i(r)$ due to changes in $f_i(0)$ is given by the Jacobian matrix with components

$$J_{ij} = \frac{\partial f_i(r)}{\partial f_j(0)} . \quad (\text{A.3})$$

To find such a component, we choose $A_j(0) = 1$ for the j of interest and 0 for the others, and then $J_{ij}(r) = A_i(r)$. Thus, for each j , the $J_{ij}(r)$ are the solution to the system of differential equations

$$J'_{ij}(r) = \frac{\partial F_i}{\partial f_k} J_{kj}(r) \quad \text{with initial conditions } J_{lj}(0) = \delta_{lj} . \quad (\text{A.4})$$

Since (A.4) holds for each j , we can consider it to be a matrix differential equation giving all components of $J_{ij}(r)$.

Let us apply this technique to the Jacobian for the differential equations given in (2.5). First we convert these equations into a set of first order equations by defining auxiliary fields $\phi'_i = \phi_{i+N}$ and rewriting (2.5) as

$$\begin{aligned} \phi'_{i+N} &= -\frac{D-1}{r} \phi_{i+N} + \frac{\partial U}{\partial \phi_j} , \\ \phi'_i &= \phi_{i+N} . \end{aligned} \quad (\text{A.5})$$

Now the problem is mapped into the form of (A.1) and we get a simple expression

$$\frac{\partial F_A}{\partial f_B} = \left(\begin{array}{c|c} \mathbf{0} & \mathbf{I} \\ \hline \partial^2 U / \partial \phi_i \partial \phi_j & -\frac{D-1}{r} \mathbf{I} \end{array} \right) \quad (\text{A.6})$$

To calculate the Jacobian we first solve the differential equations (2.5) and then evaluate (A.6) along the solutions ϕ to solve (A.4) and get $J_{AB}(r)$.

For the first and last interval we must also take account of the fact that we specify only ϕ_1 and ϕ_n , and ϕ'_1 and ϕ'_n are determined from these. Those derivatives then in turn determine the initial conditions used in shooting. Thus the Jacobian for these cases must include the effect of a change in the field value upon the derivative found by the procedures of section 4.2.

When we consider variations of ϕ_1 , we should consider changes to the Hessian matrix B_{ij} of equation (4.2), because of being evaluated at a different ϕ . But these depend on the third derivatives of the potential and are complicated to calculate. So we have ignored this effect in computing the Jacobian. This should not creating any larger problem than ignoring these same third derivatives in computing the analytic approximations.

A.2 Jacobian with respect to Δ

As described in subsection 4.3 we do not evaluate the fields at constant values of r . Instead we have an extra variable Δ which changes the value of the r_i where we apply the parameters. Fortunately, we do not need to solve extra differential equations to compute the effect of changing Δ . The matching points are

$$R_i = \{r_1 + \Delta, r_2 + \Delta, \dots, r_n + \Delta\} \quad (\text{A.7})$$

Here we show the procedure for case of $n = 4$ case, which is depicted in figure 4, with a single field. Generalization to arbitrary n and N is straightforward. First we calculate the following

Jacobian using the technique described in section A.1:

$$J = \begin{pmatrix} \frac{\partial \phi_L(r_2)}{\partial \phi(r_1)} & 0 & 0 & 0 \\ \frac{\partial \phi'_L(r_2)}{\partial \phi(r_1)} & 0 & 0 & 0 \\ 0 & \frac{\partial \phi_L(r_3)}{\partial \phi(r_2)} & \frac{\partial \phi_L(r_3)}{\partial \phi'(r_2)} & -\frac{\partial \phi_R(r_3)}{\partial \phi(r_4)} \\ 0 & \frac{\partial \phi'_L(r_3)}{\partial \phi(r_2)} & \frac{\partial \phi'_L(r_3)}{\partial \phi'(r_2)} & -\frac{\partial \phi'_R(r_3)}{\partial \phi(r_4)} \end{pmatrix}. \quad (\text{A.8})$$

When we add the new variable Δ , our Jacobian will have the same number of rows, but one more column, giving the dependence of the various parameters on Δ ,

$$J_{\text{total}} = \left(\begin{array}{c|c} J & \begin{pmatrix} \frac{\partial \phi_L(r_2)}{\partial \Delta} \\ \frac{\partial \phi'_L(r_2)}{\partial \Delta} \\ \frac{\partial \phi_L(r_3)}{\partial \Delta} - \frac{\partial \phi_R(r_3)}{\partial \Delta} \\ \frac{\partial \phi'_L(r_3)}{\partial \Delta} - \frac{\partial \phi'_R(r_3)}{\partial \Delta} \end{pmatrix} \end{array} \right). \quad (\text{A.9})$$

There are two types of effects due to Δ . First, after we solve the differential equation, changing r_i changes the place at which the solution is evaluated. Second, changing r_i changes which solution of the differential equation we use when we start from the same initial data $\phi(r_i)$ and $\phi'(r_i)$. We can propagate the new data back to the former location of r_i , changing the ϕ and ϕ' values used as initial conditions appropriately.

In all, we find six types of terms that we need to calculate:

$$\begin{aligned} \frac{\partial \phi_L(r_3)}{\partial \Delta} &= \phi'_L(r_3) - \phi'(r_2) \frac{\partial \phi_L(r_3)}{\partial \phi(r_2)} - \phi''(r_2) \frac{\partial \phi_L(r_3)}{\partial \phi'(r_2)}, \\ \frac{\partial \phi'_L(r_3)}{\partial \Delta} &= \phi''_L(r_3) - \phi'(r_2) \frac{\partial \phi'_L(r_3)}{\partial \phi(r_2)} - \phi''(r_2) \frac{\partial \phi'_L(r_3)}{\partial \phi'(r_2)}, \\ \frac{\partial \phi_L(r_2)}{\partial \Delta} &= \phi'_L(r_2) - \phi'(r_1) \frac{\partial \phi_L(r_2)}{\partial \phi(r_1)}, \\ \frac{\partial \phi'_L(r_2)}{\partial \Delta} &= \phi''_L(r_2) - \phi'(r_1) \frac{\partial \phi'_L(r_2)}{\partial \phi(r_1)}, \\ \frac{\partial \phi_R(r_3)}{\partial \Delta} &= \phi'_R(r_3) - \phi'(r_4) \frac{\partial \phi'_R(r_3)}{\partial \phi(r_4)}, \\ \frac{\partial \phi'_R(r_3)}{\partial \Delta} &= \phi''_R(r_3) - \phi'(r_4) \frac{\partial \phi'_R(r_3)}{\partial \phi(r_4)}. \end{aligned} \quad (\text{A.10})$$

The partial derivatives on the right in (A.10) are all elements of the original Jacobian J . The first derivatives at r_2 and r_3 are variables, while those at r_1 and r_4 can be computed from the analytic forms given in section 4.2. Finally, the second derivatives can be computed using the equations of motion,

$$\phi''(r_i) = U'(\phi(r_i)) - \frac{D-1}{r_i} \phi'(r_i). \quad (\text{A.11})$$

B Powell's method for solving equations

M. J. D. Powell [39] describes a method for solving multiple simultaneous equations that is a hybrid of Newton's method and gradient descent. We describe this method briefly here; for more details, see Ref. [39].

Powell’s hybrid method attempts to iteratively find the simultaneous root of a set of nonlinear functions $f_i(x_1, \dots)$. Given some current guess \mathbf{x} , the method finds some step δ such that $\mathbf{x} + \delta$ is a better approximation to the desired root. This is done by (potentially) combining two possible steps.

We first linearize the equations around the point \mathbf{x} . Newton’s method works by considering next the solution to these linearized equations. This method is quadratically convergent if one is close enough to the actual solution. But if not, the next guess can be much further from the actual solution than the previous one.

An alternative is to move in the direction which most rapidly decreases the squared error $F(\mathbf{x}) = \sum_i x_i^2$. This is a quadratic in the linearized $f_i(\mathbf{x})$, so it achieves a minimum at some distance from \mathbf{x} and we will call this direction and distance the gradient step.

Powell’s hybrid method combines these ideas as follows. It maintains at each time a desired step size Δ (in the Euclidean norm on the space of parameter values). If the step recommended by Newton’s method is shorter than Δ , Powell’s method tries to take the Newton step. If not, consider the gradient step. If it is longer than Δ , try going distance Δ in the gradient direction. If it is shorter, try a linear combination of the gradient step and the Newton step that has length Δ .

In all cases, if the trial step decreases F we take it, and adjust the step size based on how much progress we are making. If the trial fails to decrease F , we try shorter and shorter steps until we find one that does. If only an infinitesimal step decreases F , it appears that we have found a local minimum and must give up.

The method starts always with a gradient step. If the method appears to be working, it moves more and more toward Newton’s method, and eventually converges rapidly on the solution. If things are going poorly, it slowly descends the surface of F until it finds an area where it can move rapidly towards the solution (or fails at a local minimum).

In order to apply this method, we need the Jacobian $\partial f_i / \partial x_j$. Powell [39] describes techniques for maintaining an approximate Jacobian by a series of function evaluations. But here we are able to compute the Jacobian numerically, as described in Sec. A, so we do not need these techniques. As described in Sec. 4.3, we extended the method to allow more variables than functions. This has no effect at all on the gradient method: we move in the direction that most rapidly decreases F , just as before. For Newton’s method, there are now many possible steps that solve the linearized equations, and we choose the shortest of these.

C Obtaining and running the code

We have implemented the above procedures in Mathematica. The code can be downloaded from <http://cosmos.phy.tufts.edu/AnyBubble/>. There is a manual which explains how to find instanton solutions and all the options available in the code.

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